Generating Cosmological Gaussian Random Fields

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ABSTRACT

We present a generic algorithm for generating Gaussian random initial conditions for cosmological simulations on periodic rectangular lattices. We show that imposing periodic boundary conditions on the real-space correlator and choosing initial conditions by convolving a white noise random field results in a significantly smaller error than the traditional procedure of using the power spectrum. This convolution picture produces exact correlation functions out to separations of L/2, where L is the box size, which is the maximum theoretically allowed. This method also produces tophat sphere fluctuations which are exact at radii $R \leq L/4$. It is equivalent to windowing the power spectrum with the simulation volume before discretizing, thus bypassing sparse sampling problems. The mean density perturbation in the volume is no longer constrained to be zero, allowing one to assemble a large simulation using a series of smaller ones. This is especially important for simulations of Lyman-α systems where small boxes with steep power spectra are routinely used.

We also present an extension of this procedure which generates exact initial conditions for hierarchical grids at negligible cost.

Subject headings: methods: numerical — large-scale structure of universe

1.   Introduction

Cosmological N-body and hydrodynamic simulations have numerical resolution limitations imposed on both large scales comparable to the simulation box (Gelb and Bertschinger 1994, hereafter GB), as well as on small scales due to finite resolution (Hockney and Eastwood 1981). For simulations of Cold Dark Matter initial conditions, they found that for a box of width L=51.2 Mpc, the truncation of the power spectrum at the box length resulted in fluctuations on 8 Mpc spheres σ_8 which are systematically 40% lower than the analytical value. This factor of nearly 2 in error arises due to the truncation of the power spectrum while generating the initial conditions. They found that a box size

with L=100 Mpc was required to reduce the error to 10%. In cosmological applications, the actual value of σ_8 is of significant interest since it corresponds to the mass fluctuations from which a rich cluster forms. In the Press-Schechter framework (Press and Schechter 1974), cluster abundances will be statistically correct as long as σ_R is exactly modeled in a simulation, where $M = (4/3)\pi R^3 \rho_c$ is the mass of the cluster in question. Since computational cost grows at least as fast as the third power of the simulation volume at fixed physical resolution, it is desirable to use numerical discretizations which allow the most accurate representation of physical processes with the minimal simulation volume. The first purpose of this letter is to demonstrate how the initial conditions in a periodic box can be chosen to eliminate this error entirely for tophat smoothing scales which are of size up to L/4. When an ensemble of simulations is performed, their average will reflect the correct tophat fluctuation distribution.

The current trend in high-resolution simulations is to adaptively place high resolution grids in regions which are known to form high density objects (Bryan and Norman 1995, Dutta 1995, Navarro *et al.* 1995, Bartelmann and Steinmetz 1996). If this procedure is repeated recursively, one needs to be able to specify the initial conditions at very high resolution in these regions. The brute force approach needs to generate the initial conditions at high resolution everywhere, and throw out the regions which are never resolved. The convolution picture (Salmon 1996) allows a simple decomposition of the problem into multiple scales, each of which is rapidly computed using a FFT. This paper describes the optimal implementation of the convolution picture for cubical regular or hierarchical grids.

A third related problem is the question of how one might embed a small periodic simulation volume inside of a larger one. For example, one might simulate a large 1Gpc³ volume of the universe at modest resolution, and identify a region in this simulation (perhaps an extremely rich cluster or empty void) which one would like to study at higher resolution. Since perturbations on scales of even 100 Mpc are small, one might envision drawing 100 Mpc box from the large volume and only simulating the smaller volume at higher resolution. If the simulation imposes periodic boundary conditions, the procedure described in this letter will allow us to generate such a box which agrees very well with the larger box in the central regions of overlap. The converse was studied by Tolman and Bertschinger (1996), which is how to run a large simulation at high resolution given a small one. This problem also fits in the framework of the convolution picture.

The general solution to all three problems is to envision the generation of initial conditions in coordinate space instead of Fourier Space. We will initially lay down a random number at each grid point. Now gridpoints are uncorrelated with each other, and the correlator is a Dirac δ-function. Let us now convolve this initial condition with

some appropriate window $W_\rho(r)$. Convolution, being a linear process, will preserve the Gaussianity of the random field, but introduces a correlation function which is just the auto-correlator of W_ρ. Numerically, this convolution will be performed again with the aid of FFTs. Since it is so similar to the Fourier method in implementation one can ask why it would give significantly different answers. The standard discretization of the power spectrum only samples at discrete frequencies k. For small k, this error can be large, especially if the slope of the power spectrum is steep. Discretizing a periodic correlator is equivalent to convolving the power spectrum with the window function of the simulation geometry, which smoothly averages over the power spectrum in the regions were it is poorly represented. For power spectra which have significant features, for example due to baryon oscillations, this is especially important. The correlator constructed in this manner should show absolutely no error for $r < L/2$. This is the qualitative reason for the improved performance of the convolution picture.

The effect of truncating the power spectrum are particularly severe if the power spectrum is steep. As the slope n of the power spectrum $P(k) = k^n$ approaches $n \to -3$, most of the small scale top hat variance arises from large wavelength modes which are not included in the box size. For Cold Dark Matter power spectra, the slope approaches this value on small scales, and simulations of the early non-linear mass scales, for example in Lyman-α simulations, are more strongly affected by the loss of long waves (see for example Rauch *et al.* 1996 and references therein).

This letter will mathematically describe the implementation in section 2. Numerical measures of the convolution performance are given in section 3 together with a discussion of its application to generate simulations which give the correct ensemble average. In section 4 we describe how the convolution method allows the seamless adaptive generation of subpower for hierarchical grids, and how to generate consistent periodic sub-(super) boxes. Initial conditions on unstructured grids can be treated by the tree algorithm (Salmon 1996).

2. Formalism

We consider density fields $\delta(\mathbf{x})$ where $\mathbf{x} = (x, y, z)$ is a position in three dimensional Euclidean space. The *autocorrelation function* (or auto-correlator for short) is defined as $\xi(r) = < \delta(\mathbf{x})\delta(\mathbf{x} + r) >$. The density field can be transformed into Fourier space $\delta(\mathbf{k}) = V^{-1} \int \exp(-i\mathbf{k} \cdot \mathbf{x})\delta(\mathbf{x})d^3x$, where we measure the *power spectrum* $P(k) = \delta(\mathbf{k})\delta(-\mathbf{k})$. The power spectrum is also the Fourier Transform of the auto-correlator. We define the spherical tophat window function $W_T(u) = 3[\sin(u) - u\cos(u)]/u$ with which we measure the standard deviation of the density field smoothed on tophat spheres of radius

R $\sigma_R^2 = 4\pi \int P(k)W_T(kR)k^2 dk$. The *traditional discretization* to obtain a random density field is to choose a Gaussian random number for each mode $\delta(\mathbf{k})$ in Fourier space with variance $P(|\mathbf{k}|)$. For small k, the spacing of modes $\Delta k \sim 2\pi/L$, where L is the simulation box length. Where $k \sim 2\pi/L$, this sampling introduces significant coarse graining error, which we will call the *truncation error*. Within the Fourier domain, we next introduce the cubical tophat window $W_C(\mathbf{k}) = \sin(2\pi Lk_x)\sin(2\pi Lk_y)\sin(2\pi Lk_z)/[(2\pi L)^3 k_x k_y k_z]$, which reflects the simulation geometry. To implement the *convolution picture*, we define the *correlation kernel* $W_\rho(k) = \sqrt{P(k)}$. We call it a "picture" since it is equivalent to the Fourier space discretization for infinite volumes, so no new physics is introduced. Since $P(k)$ is positive, so is W_ρ, but not necessarily its inverse Fourier transform $W_\rho(\mathbf{x})$. One can verify that the auto-correlator is the auto-convolution of the correlation kernel $\xi(r) = <W_\rho(\mathbf{x})W_\rho(\mathbf{x}+r)>$. We now generate a random field with zero correlation length $\delta_0(\mathbf{x})$ and define $\delta(\mathbf{x}) = \int \delta_0(\mathbf{x}')W_\rho(\mathbf{x}-\mathbf{x}')d^3\mathbf{x}'$.

We now consider two alternatives to implement these relations on a periodic lattice. In Fourier space, periodicity means that only a discrete spectrum of modes are represented. At the modes which are represented, the traditional approach is to simply use the power spectrum $P(k)$ at those discrete intervals. Two problems arise. If the power spectrum changes significantly between successive modes, one misses the intermediate power. The extreme case would be if the power spectrum had a feature, say a peak, which did not lie on one of the discrete grid points. The other problem is that the $k = 0$ mode is now forced to be zero. We see that we really want some way of not just using the value of $P(k)$, but some average over the width of the simulation volume W_C.

In the convolution picture, we impose periodicity on the correlator. We first set the correlator equal to zero outside of the box volume, and then create periodic images. We will add a superscript $^{\mathrm{grid}}$ to indicate any quantity which has been made periodic using this convolution picture prescription. For the effective grid power spectrum, this is equivalent to replacing the simulation power by the full power spectrum convolved with W_C:

$$P^{\mathrm{grid}}(\mathbf{k}) = \int P(|\mathbf{k}'|)W_C(\mathbf{k}'-\mathbf{k})d^3\mathbf{k}'. \tag{1}$$

The effect of this convolution is biggest at small k, especially $k = 0$, where the analytic power spectrum is typically 0, but the windowed one takes on some finite value which is similar to the variance in the box simulation volume. The window function of the simulation geometry smoothly averages between the finite discrete sampling imposed by the periodic boundary conditions. Due to the anisotropy of W_C the grid power spectrum $P^{\mathrm{grid}}(\mathbf{k})$ has an angular dependence. We will discuss the effects of (1) in more detail in section 3.

3.   Errors

Figure 1 shows the ensemble averaged value of σ_8 computed using the traditional power spectrum as well as in the convolution picture. The GB estimate of σ_8 truncates the lower bound of the integral over the power spectrum in Equation (2) at $k = 2\pi/L$. The result for a model with power spectrum $\Gamma = .25$, $\sigma_8 = 1$ (Bardeen *et al.* 1998) is shown as the dotted line in the figure. In order to obtain the exact value of the periodic box σ_8, we computed the actual tophat convolution on a discrete 128^3 grid without assuming a spherical cutoff in the power spectrum. This leads to the actual values of σ_8 shown as the dashed line. The solid line from the convolution picture was generated on a 256^3 lattice taken from a code which actually computes N-body simulation initial conditions.

We notice the significant improvement in the linear theory analysis which is exact for box sizes greater than 32 h^{-1} Mpc. Even for box sizes of 16 h^{-1} Mpc, where the 8 h^{-1} Mpc spheres start wrapping around the period volume, the convolution picture has an error of only 7%. By contrast, discretizing the power spectrum introduces an error of over 60%. We notice further that the convolution picture typically *overproduces* σ_8, while truncation in Fourier space underestimates it. We can understand it as follows. The correlation function is now forced to be periodic, so instead of steadily decaying at large separations, it increases beyond the periodicity radius. We have

$$\sigma_R^2 = 4\pi \int_0^{2R} \xi(r) W_T^2(r) r^2 dr \tag{2}$$

where $W_T^2(r)$ is the convolution of the tophat kernel with itself. It is zero for $r > 2R$, so we say that it has *compact support*. Periodicity thus causes (2) to be overestimated because ξ itself is overestimated for correlators which are positive and decreasing at $r = L/2$. Truncation in Fourier space, on the other hand, usually results in an underestimate because long waves are lost.

A related problem is the box-to-box density variance. In the traditional power spectrum generation, the total density within each box is typically defined to be the cosmic mean density. In reality, this value varies even when averaged over a corresponding volume of the universe. The mean density of the box can be modeled as a change of the mean matter density Ω and incorporated in the evolution of the scale factor. This addresses one of the causes of systematically underestimating σ_8, which can result in systematic errors when simulating the abundance of virialized objects such as clusters of galaxies in finite volumes. In the convolution picture, the periodic correlator does not have zero mean, so the $k = 0$ mode will have finite power. The variance thus induced will not be exactly equal to the true variance in cubical tophats of the same volume. The difference in shown in Figure 2. We see that the variance of the whole box variance is slightly overestimated, but typically only
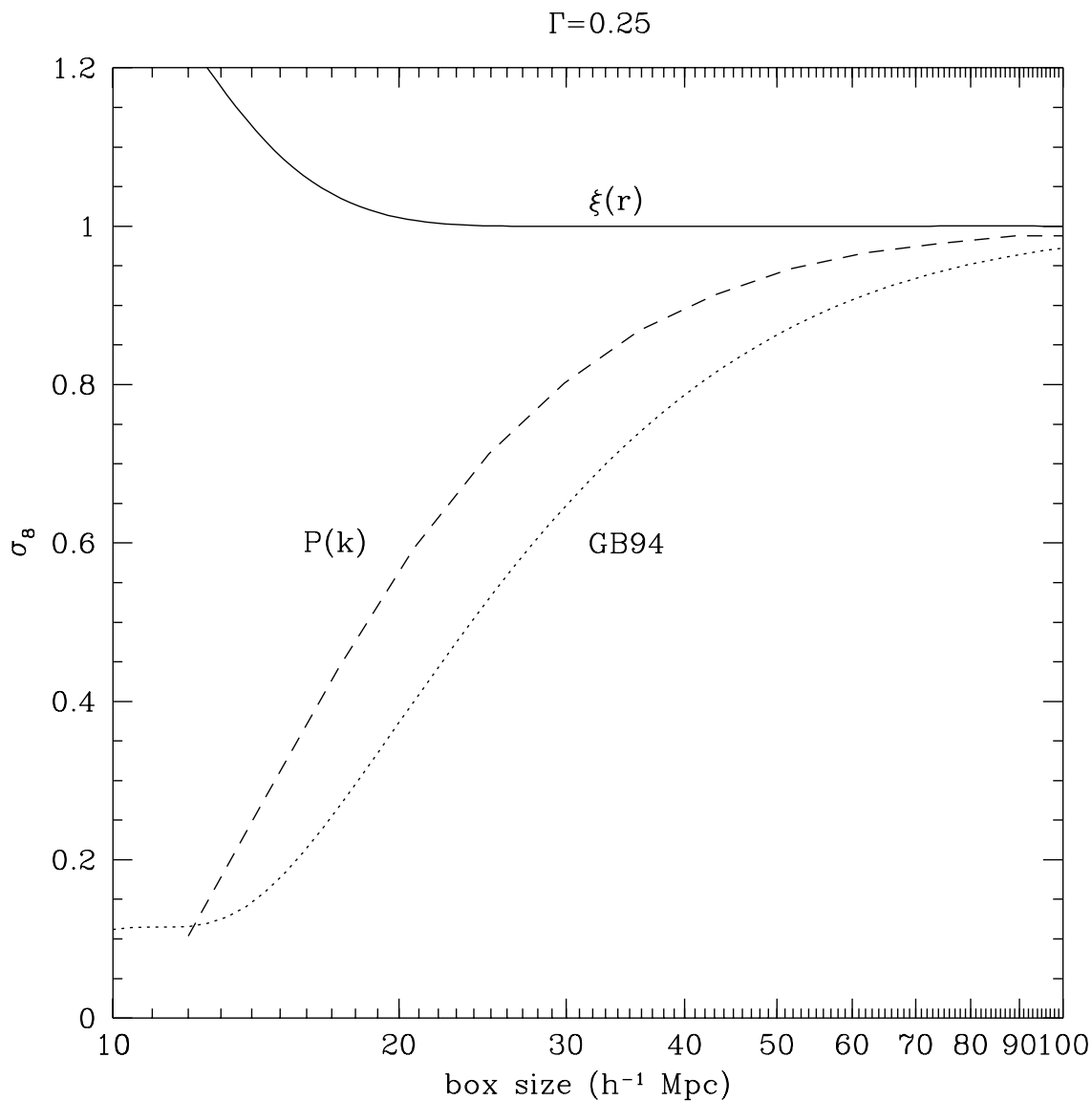
Fig. 1.— σ_8 as a function of box size using various approximations. The dotted line was computed by GB94 using a truncated power spectrum. The dashed line is the actual tophat fluctuation in a 128^3 box. The solid line was obtained using the convolution picture. The latter is exact for box sizes greater than $32\ h^{-1}$ Mpc.

by 10%. The tophat spheres of up to $R = L/4$ all have the exact variances, but the box variance itself corresponds to $R \gtrsim L/2$. The correlator is already completely determined by requiring the smaller ones to be exact, so we have no additional freedom to adjust the large scale fluctuations. Luckily the corrections are small because the dominant contribution in (2) comes from $R < L/4$.

A dual view of this picture is that the box-to-box variance is described by Equation (1) where W_C is replaced by W_C^2. One could pose the question why one doesn't simply make such a replacement for all modes. The reason is that imposing exact variances in tophat spheres which can be embedded in half the simulation width, makes Equation (1) the unique solution. If one is interested in the dynamics and abundance of bound objects, the success of the Press-Schechter ansatz argues that the top-hat spheres should be of primary importance. A potential drawback of Equation (1) is that the grid power may become negative, making it impossible to use it as a variance. On the numerical grid, one can add a constant to the numerical power spectrum to make it positive everywhere. This is equivalent to adding white noise, which shows up only in the $r = 0$ bin of the two-point correlator. In practice, for the transfer function used in this study, the effect of varying $\xi(0)$ between 0 and $\xi(\Delta r)$, the value of the correlator at one grid cell lag, did not affect measures like σ_8 by more than 1 part in 1000 even down to box sizes of 10 Mpc on a 128^3 grid. We finally note that the simulation results must be analyzed in the same way as an observational survey. The power spectrum of the simulation volume is not a true representation of the infinite volume power spectrum. It is instead a windowed sample, which must be taken into account during statistical analysis.

4. Subgrid Power

One direct advantage of the convolution picture is its adaptability to arbitrary domains. We first consider the situation where we want to add power on subgrid scales. Consider a fine rectangular grid (heavy lines) which is superposed on a coarser outer grid as shown in figure 3. Also shown is the dotted extended fine grid, which is larger than the fine grid by an amount parameterized by R. We will assume that a random initial condition was already generated on the coarse grid.

We first note that the correlation kernel can always be decomposed into a sum of two kernels $W_\rho = W_R + W_R'$ where we can choose

$$W_R(r) = \begin{cases} W_\rho(r) & \text{if} \quad r > R \\ W_\rho(R) & \text{if} \quad r \leq R \end{cases} \tag{3}$$
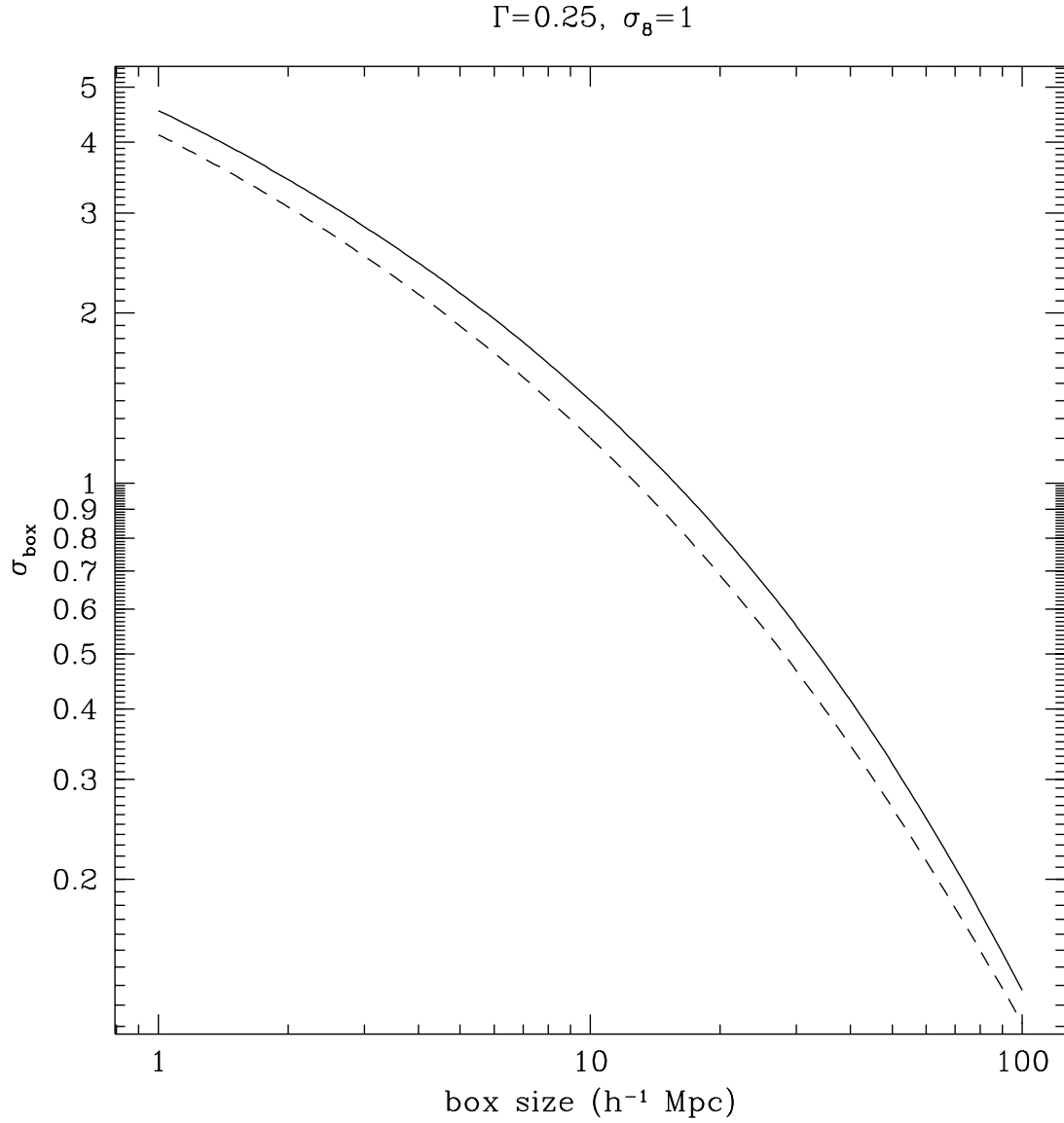
Fig. 2.— The standard deviation of the box density using the correlator (solid) and the exact value (dashed). The normalization chosen is $\sigma_8 = 1$ and $\Gamma = 0.25$. The convolution picture always slightly overestimates the box-to-box variance (see text).
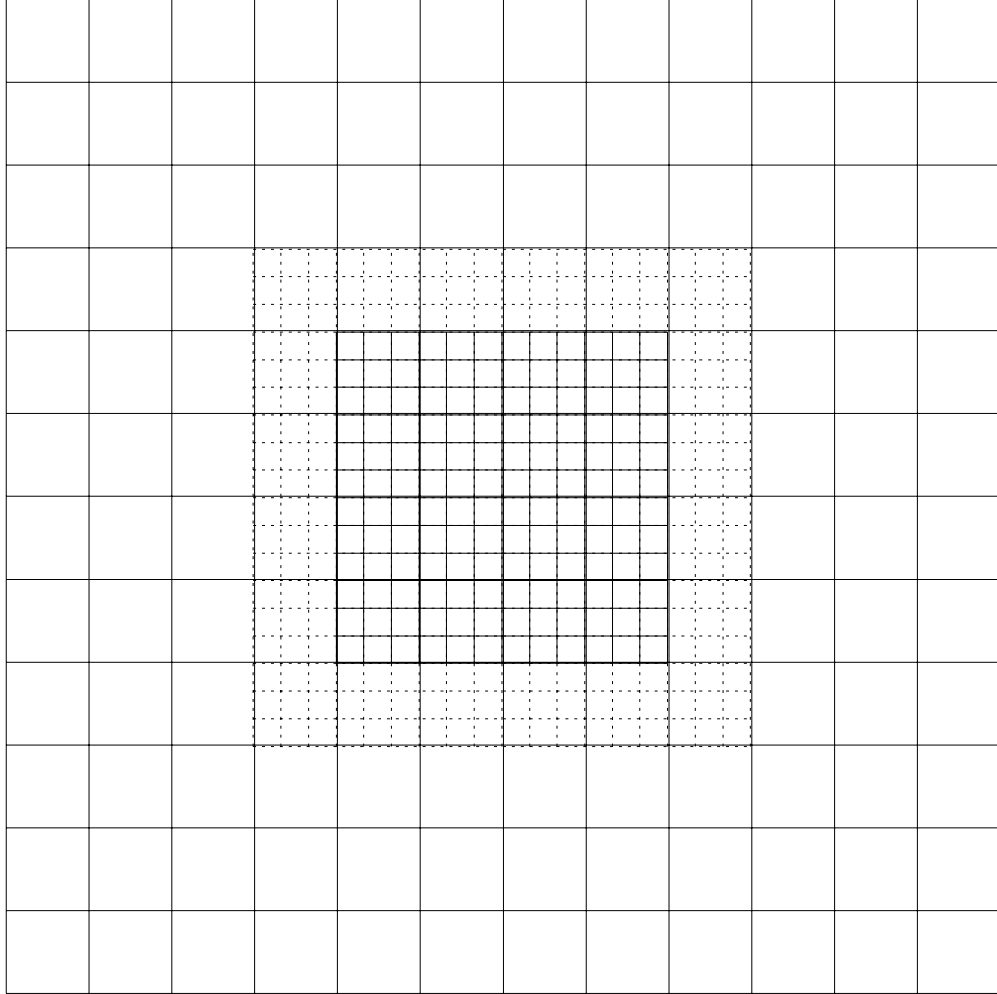
Fig. 3.— Hierarchical mesh. The dotted lines are the buffer zones on which fine mesh initial seeds need to be chosen such that a seamless period-free convolution can be applied.

By deduction, W'_R will be zero for $r > R$, i.e. it has compact support. The correlation kernels are obtained by taking the square root of the periodic correlator $W_{\rho,\text{grid}}(k) = \sqrt{\xi_{\text{grid}}(k)}$ in Fourier space and transforming back to coordinate space.

We will first generate initial conditions on the whole coarse grid with W_R. We linearly project these values onto the fine grid. This we will call $\delta_1^{\text{fine}}(\mathbf{x})$. We then Fourier Transform all the white noise conditions $\delta_0(\mathbf{k})$ into coordinate space on the coarse grid $\delta_0(\mathbf{x})$, and also project these seeds onto the extended fine grid which we call $\delta_0^{\text{fine}}(\mathbf{x})$. Let N be the refinement factor. The fine grid is now constant on cubicles with N^3 elements. For each cubicle, we will add random white noise on each grid cell of variance N^3 times the original white noise variance, subject to the constraint that the average must be the coarse cell value. Call the white noise field δ_2^{fine}. To implement the constraint, we subtract from each cubicle its mean and add the coarse cell value. Call the resultant density field $\tilde{\delta}_2^{\text{fine}}$. We now convolve this field with W'_R and add it to δ_1^{fine}. Since W'_R is only nonzero for $r < R$, we only need to add a buffer zone of width R to the fine grid to obtain a full fine grid power spectrum. The actual choice of R depends on how smoothly one wishes to interpolate from coarse grid power to fine grid power. A typical choice of 2 grid cells should interpolate reasonably smoothly.

In the language of multigrid (Press *et al.* 1992), we can summarize this procedure in terms of the prolongation operator $\mathcal{P}$, the restriction operator $\mathcal{R}$ and the convolution operator $*$. $\mathcal{P}$ maps from the coarse grid to the fine grid by using the nearest grid point. $\mathcal{R}$ does the converse map by averaging over the contained subdomain. We define the constrained fine grid as a white noise random field with variance $< (\delta_2^{\text{fine}})^2 >= N^3 < \delta_0^2 >$, and $\delta_0 = \mathcal{R}\delta_1^{\text{fine}}$. Using the new operators, we can implement the constrained subpower as $\tilde{\delta}_2^{\text{fine}} = \mathcal{P}\delta_0 + \delta_2^{\text{fine}} - \mathcal{P}\mathcal{R}\delta_2^{\text{fine}}$. This gives us a compact prescription for the new fine grid power:

$$\delta^{\text{fine}} = \mathcal{P}W_R * \delta_0 + W'_R * (\mathcal{P}\delta_0 + \delta_2^{\text{fine}} - \mathcal{P}\mathcal{R}\delta_2^{\text{fine}}). \tag{4}$$

The same procedure can be used to embed a high resolution small volume simulation inside a larger grid. The reverse of the procedure above will be used. We build the large grid white noise field from the small grid using the restriction operator $\delta_0 = \mathcal{R}\delta_0^{\text{fine}}$ in the region of overlap, and fill the rest of the volume with new random numbers. These are then convolved with the appropriate window W_ρ. If the power on the grid scale of the small volume simulation was moderately small, the two grids will be consistent with each other in the central regions of overlap. The converse operation corresponds to cutting out a small volume from a larger one, and simulating the small volume at high resolution with periodic boundary conditions. This is straightforward if we perform the cutting on the white noise grid $\delta_0(\mathbf{x})$, and then apply the periodic convolution on the smaller white noise grid.

5. Conclusion

Numerical simulations introduce unphysical truncation errors on two scales: the grid scale and the box length. At the grid scale, errors are dominated by the computation of forces and field evolution. At the box scale, currently simulations are often limited by the discretization of the power spectrum. For many problems in cosmology, this limit can be improved when described in the picture of Press-Schechter structure formation.

We have shown how initial conditions should be generated for cosmological simulations utilizing small periodic box volumes. A box is considered small if the variance on the box scale is not small, typically greater than 10%. For CDM models, this means any box smaller than $\sim 50h^{-1}$ Mpc. By discretizing the correlator instead of the power spectrum, we obtain more accurate estimates of tophat variances and correlators, which are often the primary target of study in N-body simulations.

We have also applied this approach to decompose the correlation kernel into a long range and short range part, allowing us to add small scale power for hierarchical subgrids without imposing periodicity on the subgrid subpower. This procedure generalizes to embedding small periodic simulations inside of larger ones and vice versa.

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